

Abstract

A Binary-Encounter-Bethe approach to simulate DNA damage by the direct effect

By Ianik Plante¹ and Francis A. Cucinotta²

¹Universities Space Research Association, Houston, TX, 77058

²NASA Johnson Space Center, Houston, TX, 77058

The DNA damage is of crucial importance in the understanding of the effects of ionizing radiation. The main mechanisms of DNA damage are by the direct effect of radiation (e.g. direct ionization) and by indirect effect (e.g. damage by 'OH radicals created by the radiolysis of water). Despite years of research in this area, many questions on the formation of DNA damage remains. To refine existing DNA damage models, an approach based on the Binary-Encounter-Bethe (BEB) model was developed [1]. This model calculates differential cross sections for ionization of the molecular orbitals of the DNA bases, sugars and phosphates using the electron binding energy, the mean kinetic energy and the occupancy number of the orbital. This cross section has an analytic form which is quite convenient to use and allows the sampling of the energy loss occurring during an ionization event. To simulate the radiation track structure, the code RITRACKS developed at the NASA Johnson Space Center is used [2]. This code calculates all the energy deposition events and the formation of the radiolytic species by the ion and the secondary electrons as well. We have also developed a technique to use the integrated BEB cross section for the bases, sugar and phosphates in the radiation transport code RITRACKS. These techniques should allow the simulation of DNA damage by ionizing radiation, and understanding of the formation of double-strand breaks caused by clustered damage in different conditions.

References:

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